

Thermodynamic aspects of information transfer in complex dynamical systems

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From the Horowitz-Esposito stochastic thermodynamical description of information flows in dynamical systems [J. M. Horowitz and M. Esposito, Phys. Rev. **X4**, 031015 (2014)], it is known that while the second law of thermodynamics is satisfied by a joint system, the entropic balance for the subsystems is adjusted by a term related to the mutual information exchange rate between the two subsystems. In this article, we present a quantitative discussion of the conceptual link between the Horowitz-Esposito analysis and the Liang-Kleeman work on information transfer between dynamical system components [X. S. Liang and R. Kleeman, Phys. Rev. Lett. **95**, 244101 (2005)]. In particular, the entropic balance arguments employed in the two approaches are compared. Notwithstanding all differences between the two formalisms, our work strengthens the Liang-Kleeman heuristic balance reasoning by showing its formal analogy with the recent Horowitz-Esposito thermodynamic balance arguments.

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I. INTRODUCTION

There are several factors that drive the merging of information-theoretic methods to study the physics of complex dynamical systems. For instance, an important motivation is provided by the fact that the interacting components (that is, subsystems) of physical systems generate information at a nonzero rate [1] and exchange information as they influence each other [2]. A quantitative description for the processes of production, gathering, and exchange of information can be provided by means of the concept of entropy. In turn, the notions of information and entropy lead naturally to thermodynamic arguments [3]. Indeed, the second law of thermodynamics is a fundamental guiding principle that imposes fundamental limits to the amount of information that can be gathered [4] and/or exchanged [5] between interacting components of a physical system.

The interest in describing and, to a certain extent, understanding the dynamics of information transport in complex

systems is justified by the important role that information transfer analysis has in detecting asymmetry in the interaction of subsystems [1], in predicting the weather [6], in controlling a system [7, 8], in inferring causal structures [9, 10], and, from a more conceptual standpoint, in investigating the thermodynamics of Maxwell’s demon [11–13].

A convenient way to understand the relation between information and thermodynamics is by investigating the manner in which information flow affects the thermodynamics of a system. Two important quantities in information theory and thermodynamics are given by the rate of mutual information [14] and the thermodynamic entropy production [15–17], respectively. In particular, entropy production is a central physical observable in stochastic thermodynamics [17, 18], a framework to study systems far from equilibrium. Entropic rates of information-theoretic nature, instead, are central quantities in information theory. Therefore, it seems reasonable to expect that the investigation of the relation between thermodynamic and information-theoretic entropic rates can pave the way to a better understanding of the link between information and thermodynamics. Indeed, this reasonable expectation has been already explicitly tested in a quantitative manner in several works in the literature [19–21]. To the best of our knowledge, one of the first attempts to investigate the thermodynamics aspects of information flow with special regard to the inference of causal structures was presented in [22], where a version of the second law of thermodynamics was used to characterize the thermodynamic cost for information flow in a system defined by a pair of Brownian particles, each coupled to a thermal bath at different temperatures. A similar type of hybrid information-theoretic and statistical physics approach, including reasonings based upon the second law, to the study of information flow in interacting systems has been recently discussed by Hartich-Barato-Seifert and Horowitz-Esposito in Refs. [23] and [2], respectively. More specifically, in [22] entropic rate is defined as the time derivative of the time-delayed mutual information and is used to characterize the information flow between two Brownian particles coupled to different heat baths, as mentioned earlier. In [23], entropic rate is defined as the entropy reduction rate of a subsystem due to its coupling to the other subsystem composing the bipartite system and is used to show that Maxwell’s demon can be realized in terms of a bipartite Markov process. Finally, in [2] entropic rate is defined as the time derivative of the mutual information and is used to investigate the thermodynamics of information flow between two interacting subsystems of a Markovian bipartite system.

The notion of entropy rate in information transport mechanisms is not uniquely defined in the literature but it is not the scope of this article to provide a review of such diverse definitions. Instead, inspired by the works in [2, 22, 23], we focus on two main points in this article. First, we point out the conceptual link between the Liang-Kleeman notion of information transfer [6] and the Horowitz-Esposito notion of information flow [2]. This allows us to avoid some

heuristic arguments in the Liang-Kleeman approach and replace them with thermodynamic reasoning. This first point sets the Liang-Kleeman analysis on more foundational grounds and, in addition, exhibits its similarity with the Horowitz-Esposito thermodynamic analysis of information flow. Second, we compare the foundationally strengthened Liang-Kleeman notion of information transfer with that provided by Schreiber, after having briefly discussed the physical [24] and thermodynamical [25] interpretations of the latter. This second point improves our understanding of the differences between the two notions from a more fundamental point of view [22].

The layout of this article is as follows. In Sec. II, we reexamine the entropic aspects of both the Liang-Kleeman and the Horowitz-Esposito approaches. In Sec. III, we strengthen the Liang-Kleeman heuristic entropic balance arguments by emphasizing the formal analogies between the two approaches. We also compare such thermodynamically strengthened information transfer measure with the thermodynamic interpretation of Schreiber's transfer entropy. Finally, in Sec. IV we present our conclusive remarks.

II. CONSERVATION OF PROBABILITY

The transport of a conserved quantity is described by a continuity equation whose differential form is given by [26],

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \vec{j} = 0, \quad (1)$$

where ρ denotes the volume density of the conserved quantity and \vec{j} is the ordinary vector flux of the conserved quantity. In classical electrodynamics, for instance, the electric charge is the conserved quantity, ρ is the electric charge density, and \vec{j} is the electric current density [27]. A similar line of reasoning appears in fluid dynamics, thermodynamics, and quantum theory where the electric charge is replaced with mass, heat, and probability distributions, respectively. A continuity equation associated to the conservation of probability is the fundamental starting point of discussion in both the Liang-Kleeman and the Horowitz-Esposito approaches to information transfer and information flow.

A. The Liang-Kleeman approach: Heuristic arguments

The Liang-Kleeman approach can be applied to both deterministic and stochastic systems of arbitrary finite dimensionality, either discrete or continuous. For a recent comprehensive review of the Liang-Kleeman approach, we refer to [28]. For the latest developments on this approach, we refer instead to [29]. In this article, our discussion is based upon the working hypotheses of the original work presented in [6] which contains the essence of the philosophy of the Liang-Kleeman approach. Specifically, we shall be considering a two-dimensional continuous and deterministic

autonomous system with *a priori* knowledge of the dynamics,

$$\frac{d\vec{x}}{dt} = \vec{F}(\vec{x}), \quad (2)$$

where $\vec{x} = (x_1, x_2)$ belongs to the state space $\Omega = \Omega_1 \times \Omega_2$ and $\vec{F} = (F_1, F_2)$ with $F_i = F_i(x_1, x_2)$ for any $i = 1, 2$ is the (known) flow vector. The sample values (x_1, x_2) are associated to a stochastic process $\vec{X} = (X_1, X_2)$ with (known) joint probability density distribution at time t given by $\rho = \rho(x_1, x_2, t)$. The vector flux \vec{j} equals $\rho\vec{F}$ and the continuity equation associated with Eq. (2) becomes,

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot (\rho\vec{F}) = 0. \quad (3)$$

Assuming that ρ vanishes at the boundaries, after some suitable algebraic manipulations of Eq. (3), it is found that the temporal rate of change of the joint entropy of X_1 and X_2 ,

$$H(t) \stackrel{\text{def}}{=} - \int_{\Omega} \int \rho \log \rho dx_1 dx_2, \quad (4)$$

satisfies the relation [6],

$$\frac{dH}{dt} = \mathbb{E}(\vec{\nabla} \cdot \vec{F}). \quad (5)$$

The base of the logarithm in Eq. (4) determines the units used for measuring information: bits and nats for base-2 and base- e , respectively. Equation (5) states the dH/dt equals the expectation value of the divergence of the flow vector \vec{F} ,

$$\mathbb{E}(\vec{\nabla} \cdot \vec{F}) \stackrel{\text{def}}{=} \int_{\Omega} \int \rho (\vec{\nabla} \cdot \vec{F}) dx_1 dx_2. \quad (6)$$

To describe the decomposition of the various mechanisms responsible for the joint and individual temporal rates of changes of entropies of X_1 , X_2 , and (X_1, X_2) in terms of information transfers, Liang and Kleeman employ a very clever heuristic argument. First, following the very same line of reasoning and working hypotheses used to obtain Eq. (5), they compute both dH_1/dt and dH_2/dt where H_i denotes the entropy of X_i defined in terms of ρ_i obtained from ρ after marginalizing over the degree of freedom j with $j \neq i$. Second, they observe that if X_2 is frozen and X_1 evolves on its own, its entropic rate of change would be equal to $\mathbb{E}(\partial F_1 / \partial x_1)$. In the presence of interacting processes X_1 and X_2 they find that,

$$\frac{dH_1}{dt} \neq \mathbb{E}\left(\frac{\partial F_1}{\partial x_1}\right) \stackrel{\text{def}}{=} \frac{dH_1^*}{dt}. \quad (7)$$

Therefore, they arrive at the conclusion that the difference between dH_1/dt and $\mathbb{E}(\partial F_1/\partial x_1)$ must equal the rate of entropy transfer from X_2 to X_1 , and define transfer entropy as

$$T_{2 \rightarrow 1} \stackrel{\text{def}}{=} \frac{dH_1}{dt} - \frac{dH_1^*}{dt} = - \int_{\Omega} \int \rho_{2|1}(x_2|x_1) \frac{\partial(\rho_1 F_1)}{\partial x_1} dx_1 dx_2, \quad (8)$$

where $\rho_{2|1}(x_2|x_1) \stackrel{\text{def}}{=} \rho(x_1, x_2, t) / \rho_1(x_1, t)$. Observe that combining Eqs. (5), (7), and (8), we obtain

$$\frac{dH_1}{dt} + \frac{dH_2}{dt} = \frac{dH}{dt} + T_{1 \rightarrow 2} + T_{2 \rightarrow 1}. \quad (9)$$

At this juncture we make the following remarks. First, when a flow is additive, matter has to be lost in one component of the system in order for another component to receive it. However, information does not have to be lost in one component in order for another component to receive it. A key difference between flow of matter and flow of information is encoded into the asymmetry of the latter. Specifically, we note that if $F_1 = F_1(x_1)$ and does not depend on x_2 , we have $T_{2 \rightarrow 1} = 0$ and there is no information transfer from X_2 to X_1 . As a result of the asymmetric nature of information transfer however, this does not necessarily imply that $T_{1 \rightarrow 2} = 0$. We point out that the idea of frozen variables also appears in the framework of bipartite networks [19] where one considers Markov processes with states that are specified by two variables. In a transition between states, only one of the variables can change while the other one is kept fixed. A few recent and interesting applications of such bipartite network formalism applied to stochastic modeling for cellular and biochemical sensing appear in Refs. [20] and [21], respectively. Second, the physical consistency of the Liang-Kleeman approach with the Schreiber work [1] (see also Section III) can be explained as follows. In the former approach, a direction of the phase space is frozen in order to extract information transfer. In the latter, the transition probabilities are essentially obtained from joint probabilities by fixing one component of the joint system. Third, a conserved information-theoretic charge can be defined as,

$$Q(t) \stackrel{\text{def}}{=} H(t) - \int^t E(\vec{\nabla} \cdot \vec{F}) dt'. \quad (10)$$

In general, $Q(t)$ is not an additive quantity and it becomes so if one assumes $\rho = \rho_1 \rho_2$, $F_1 = F_1(x_1)$, and $F_2 = F_2(x_2)$. In other words, the conserved charge $Q(t)$ is additive and equals $Q_1(t) + Q_2(t)$ if and only if there is no information flow between the components X_1 and X_2 of the joint system (X_1, X_2) . We therefore conclude that the presence of information transfers between the components of a complex system is incompatible with the additivity of a conserved information-theoretic charge.

B. The Horowitz-Esposito approach: Thermodynamic arguments

The second law of thermodynamics states that the entropy of an isolated macroscopic system cannot decrease in time [30]. If fluctuation effects are also taken into account, it is possible to provide a new version of the second law and, more generally, a new thermodynamic description for small systems. Such a framework is known as stochastic thermodynamics [17, 18, 31]. In Ref. [23], being within the framework of stochastic thermodynamics, Hartich-Barato-Seifert have investigated various second-law-like inequalities valid for bipartite systems. In particular, they have provided an especially clear thermodynamical interpretation of Maxwell's demon. Specifically, they have considered a bipartite system (xy -system) where Maxwell's demon is one of the subsystems (y -system) that affects the other subsystem (x -system) used to extract work from a heat bath. Here we focus on the stochastic thermodynamical formalism used in [2] by Horowitz and Esposito to characterize how information flow influences the thermodynamics of a system described by a probability distribution that evolves according to a Markovian master equation [32] (or, more specially, a Fokker-Planck equation [33]).

In what follows, we limit our discussion to bipartite thermodynamics and information flow [2]. For a very recent analysis extended to multipartite flow, we refer to [5]. Specifically, consider a Markovian system (X, Y) described by a joint probability distribution $p(x, y)$ that evolves according to a master equation,

$$\frac{dp(x, y)}{dt} - \sum_{x', y'} \left[W_{x, x'}^{y, y'} p(x', y') - W_{x', x}^{y', y} p(x, y) \right] = 0, \quad (11)$$

where $W_{x, x'}^{y, y'}$ is the transition rate (matrix) at which the system (X, Y) jumps from (x', y') to (x, y) . An important working hypothesis in [2] is the so-called bipartite assumption according to which the fluctuations (noises) in each subsystem X and Y are independent. Although these fluctuations are not required to be generated by distinct thermodynamics reservoirs, Horowitz and Esposito employ this additional assumption for the sake of simplicity of exposition of their original argument. Equation (11) can be recast as a continuity equation as in Eq. (1) since probability is conserved. To do so, the current (probability flux) J flowing from (x', y') to (x, y) is defined as,

$$J_{x, x'}^{y, y'} \stackrel{\text{def}}{=} W_{x, x'}^{y, y'} p(x', y') - W_{x', x}^{y', y} p(x, y). \quad (12)$$

Combining Eqs. (11) and (12), the continuity equation becomes

$$\frac{dp(x, y)}{dt} - \sum_{x', y'} J_{x, x'}^{y, y'} = 0. \quad (13)$$

A key point in the Horowitz-Esposito approach that plays an essential role in our comparison with the Liang-Kleeman work is the exploitation of the bipartite structure in order to split the current $J_{x, x'}^{y, y'}$ into two separate flows, $J_{x, x'}^y$

(the current from x' to x along y) and $J_x^{y, y'}$ (the current from y' to y along x), in such a manner that

$$\sum_{x', y'} J_{x, x'}^{y, y'} \stackrel{\text{def}}{=} \sum_{x'} J_{x, x'}^y + \sum_{y'} J_x^{y, y'}. \quad (14)$$

Equation (14) implies that the flow in the joint (X, Y) -direction is the sum of two separate flows, one in the X -direction and one in the Y -direction. The reasoning of Horowitz and Esposito goes as follows. They are interested in describing how the information flow between the subsystems X and Y is linked to the thermodynamics of the joint system (X, Y) . First, they observe that the second law of thermodynamics applied to (X, Y) requires that [32],

$$\dot{S}_i = d_t S^{XY} + \dot{S}_r \geq 0, \quad (15)$$

where \dot{S}_i is the irreversible entropy production rate, \dot{S}_r is the entropy rate flowing to the environment, and $d_t S^{XY}$ denotes the time derivative of the joint (Shannon) entropy of (X, Y) . Second, they note that Eq. (15) does not explain the manner in which information flows between X and Y . To achieve this goal, they point out that \dot{S}_i , $d_t S^{XY}$, and \dot{S}_r are linear functionals of the currents, that is, they are flows. Then, in analogy to the splitting of the current as in Eq. (14), they decompose any current functional $\mathcal{A}[J]$ as,

$$\mathcal{A}[J] = \mathcal{A}^X + \mathcal{A}^Y. \quad (16)$$

The quantities \mathcal{A}^X and \mathcal{A}^Y denote the variations in the X -direction and Y -direction of $\mathcal{A}[J]$, respectively. In particular, we find

$$\dot{S}_i = \dot{S}_i^X + \dot{S}_i^Y, \text{ and } \dot{S}_r = \dot{S}_r^X + \dot{S}_r^Y. \quad (17)$$

Using Eq. (17), recalling the information-theoretic relation $S^{XY} = S^X + S^Y - I$ between joint entropy S^{XY} and mutual information I [14],

$$I \stackrel{\text{def}}{=} \sum_{x, y} p(x, y) \log \left[\frac{p(x, y)}{p(x)p(y)} \right], \quad (18)$$

and defining the so-called information flow as [2],

$$d_t I \stackrel{\text{def}}{=} \dot{I}^X + \dot{I}^Y, \quad (19)$$

it follows after some simple algebra that Eq. (15) can be decomposed into two equations,

$$\dot{S}_i^X = d_t S^X + \dot{S}_r^X - \dot{I}^X \text{ and } \dot{S}_i^Y = d_t S^Y + \dot{S}_r^Y - \dot{I}^Y, \quad (20)$$

respectively. Observe that combining Eqs. (15), (17), and (20), we obtain

$$d_t S^X + d_t S^Y = d_t S^{XY} + \dot{I}^X + \dot{I}^Y. \quad (21)$$

The two relations in Eq. (20) and especially the reasoning underlying their derivation represent the main result provided by Horowitz and Esposito that we are concerned with in this article.

III. A THERMODYNAMIC COMPARISON

In 2000, Schreiber formulated the current broadly accepted information-theoretic notion of transfer entropy [1]. Transfer entropy is a measure of time-asymmetric information transfer between jointly distributed random vectors associated with time series observations. For an interesting outline of general differences between transfer entropy and information flow defined via a time-shifted mutual information, we refer to [22]. For relatively recent thermodynamic interpretations of transfer entropy, we refer to [24, 25].

In what follows, we compare the thermodynamic interpretation of Schreiber's transfer entropy as presented in [24, 25] with the Liang-Kleeman measure of information transfer after having emphasized its formal analogy with the Horowitz-Esposito thermodynamic formalism.

A. The Liang-Kleeman approach: Thermodynamic arguments

Recall that the mutual information I between X_1 and X_2 is formally defined as [14],

$$I(t) \stackrel{\text{def}}{=} \int_{\Omega} \int \rho \log \left(\frac{\rho}{\rho_1 \rho_2} \right) dx_1 dx_2, \quad (22)$$

and equals,

$$I(t) = H_1(t) + H_2(t) - H(t). \quad (23)$$

Differentiating both sides of Eq. (23) with respect to time, we obtain

$$d_t I = d_t H_1 + d_t H_2 - d_t H. \quad (24)$$

By combining Eq. (9) and (24), we find

$$d_t I = T_{1 \rightarrow 2} + T_{2 \rightarrow 1}, \quad (25)$$

where I is defined in Eq. (22) and $T_{1 \rightarrow 2}$ in Eq. (8). After having reexamined both the Horowitz-Esposito and the Liang-Kleeman approaches, the similarities between the two approaches become almost self-evident. Specifically, Eqs. (3), (9), and (25) within the Liang-Kleeman approach correspond to Eqs. (13), (21), and (19) within the Horowitz-Esposito approach, respectively. Due to these conceptual and mathematical analogies, the heuristic entropic balance

arguments in [6] are automatically supported by the thermodynamically grounded entropic balance arguments as presented in [2]. One of our main contributions in this article is pointing out these hidden connections after a critical reconsideration of both approaches. We emphasize that the structure of Eq. (25) is similar to that of Eq. (B.5) in [23]: the time derivative of mutual information in Eq. (18) and the Liang-Kleeman definition of transfer entropy in Eq. (8) are replaced in [23] by the continuous time rate of mutual information and the continuous time version of Schreiber's transfer entropy, respectively.

B. The Schreiber approach: Thermodynamic arguments

The problem addressed by Schreiber was the following: given time series observations associated with interacting subsystems of a complex system, quantify how information produced by an individual subsystem is exchanged with another subsystem. To address this problem, Schreiber proposed an information-theoretic measure containing both dynamical and directional information. To incorporate aspects of the dynamics of information transport into the measure, Schreiber considered transition rather than static probabilities. Subsystems are assumed to be modeled in terms of stationary Markov processes. A Markov process I is of order k if the conditional probability to find I in the state i_{n+1} does not depend on the state i_{n-k} ,

$$p(i_{n+1} | i_n, \dots, i_{n-k+1}) = p(i_{n+1} | i_n, \dots, i_{n-k}), \quad (26)$$

where for notational simplicity we define $i_n^{(k)} \stackrel{\text{def}}{=} (i_n, \dots, i_{n-k+1})$. Ignoring static correlations due to common history, transfer entropy is able to detect the directed exchange of information between two subsystems by measuring the deviation from the generalized Markov property,

$$p(i_{n+1} | i_n^{(k)}) = p(i_{n+1} | i_n^{(k)}, j_n^{(l)}). \quad (27)$$

In the absence of information transfer from J to I , the state of J has no influence on the transition probabilities on system I . Transfer entropy quantifies the departure from the assumption in Eq. (27) and is defined as

$$T_{J \rightarrow I} \stackrel{\text{def}}{=} \sum_{i_{n+1}, i_n^{(k)}, j_n^{(l)}} p(i_{n+1}, i_n^{(k)}, j_n^{(l)}) \log \left[\frac{p(i_{n+1} | i_n^{(k)}, j_n^{(l)})}{p(i_{n+1} | i_n^{(k)})} \right]. \quad (28)$$

Noting that $p(i, j, k) = p(i | j, k) p(j, k) = p(i, j | k) p(k)$, after some simple algebraic manipulations, it is found that the transfer entropy in Eq. (28) can be rewritten as,

$$T_{J \rightarrow I} = \Delta s_{I|J} - \Delta s_I, \quad (29)$$

where the entropy rates $\Delta S_{I|J}$ and ΔS_I are given by,

$$\Delta S_{I|J} \stackrel{\text{def}}{=} \sum_{i_{n+1}, i_n^{(k)}, j_n^{(l)}} p(i_{n+1}, i_n^{(k)}, j_n^{(l)}) \left[\log p(i_{n+1}, i_n^{(k)} | j_n^{(l)}) - \log p(i_n^{(k)} | j_n^{(l)}) \right], \quad (30)$$

and

$$\Delta S_I \stackrel{\text{def}}{=} \sum_{i_{n+1}, i_n^{(k)}} p(i_{n+1}, i_n^{(k)}) \left[\log p(i_{n+1}, i_n^{(k)}) - \log p(i_n^{(k)}) \right], \quad (31)$$

respectively. From Eq. (29), one concludes that the transfer entropy from the process J to the process I equals the difference between the entropy rate in I (under the condition J) and the entropy rate in I . This physical interpretation of transfer entropy was originally proposed in [24]. In addition, in Ref. [24] Ito and Sagawa employed the notion of transfer entropy as defined by Schreiber in their generalized version of the second law of thermodynamics. They showed that the entropy production in a single system J interacting with multiple other systems in $\mathcal{K} = \{K_1, \dots, K_N\}$ is bounded by the information flow between these systems. Specifically, modeling the interacting systems by means of a Bayesian network [34], they showed that

$$\langle \Delta I \rangle - \langle \sigma \rangle \leq \sum_{l=1}^N T_{J \rightarrow K_l}, \quad (32)$$

where $\langle \Delta I \rangle \stackrel{\text{def}}{=} \langle I_{\text{fin}} \rangle - \langle I_{\text{ini}} \rangle$ is the difference between the ensemble averages of the final and initial correlations between J and the other subsystems in \mathcal{K} (that is, the mutual information exchanged between the systems J and \mathcal{K}), $\langle \sigma \rangle$ is the ensemble average of the entropy production σ of subsystem J , and $T_{J \rightarrow K_l}$ is the transfer entropy that characterizes the information transfer from J to K_l . For further technical details, we refer to [24]. We also remark that, inspired by the fluctuation relation for causal networks obtained in [24] and using the concept of transfer entropy in the continuous time limit [19], Barato-Hartich-Seifert have recently presented a similar fluctuation relation for a stochastic trajectory of a bipartite system [23].

In what follows, we shall focus on the thermodynamic interpretation of Schreiber's transfer entropy as proposed by Prokopenko *et al.* in Ref. [25]. The Prokopenko *et al.* approach can be synthesized as follows. For the sake of simplicity, consider a joint system (X, Y) . For each subsystem, the variation of entropy ΔS equals the sum of the entropy change caused by interactions with the surrounding ΔS_{ext} and the internal entropy production σ inside the system itself. Therefore,

$$\Delta S = \sigma + \Delta S_{\text{ext}}. \quad (33)$$

Two assumptions are employed. First, the conditional probability $p(x_{n+1} | x_n)$ is related to the transition probability of the system's reversible state change. Second, the conditional probability $p(x_{n+1} | x_n, y_n)$ is related to the transition

probability of the system's possibly irreversible internal state change, due to the interactions with the external surroundings. Furthermore, assuming a Boltzmann entropic expression for the Shannon entropy, Prokopenko *et al.* arrive at the proportionality between local transfer entropy $t_{Y \rightarrow X}$ and external entropy production ΔS_{ext} in the additional working hypothesis of small fluctuations near equilibrium [25],

$$t_{Y \rightarrow X}(n+1) \propto -\Delta S_{\text{ext}}^X, \quad (34)$$

where

$$t_{Y \rightarrow X}(n+1) \stackrel{\text{def}}{=} \log \left[\frac{p(x_{n+1} | x_n, y_n)}{p(x_{n+1} | x_n)} \right], \quad (35)$$

and transfer entropy $T_{Y \rightarrow X}$ in Eq. (29) is the expectation value $\langle t_{Y \rightarrow X}(n+1) \rangle$ of $t_{Y \rightarrow X}$ at each time step n . Considering Eq. (33) for both subsystems, using Eq. (34) and setting Boltzmann's constant k_B equal to one (the proportionality factor in Eq. (34) is given by $k_B \ln 2$ when entropy is given in units of nats), it is determined that

$$\sigma^X + \sigma^Y = \Delta S + [t_{Y \rightarrow X}(n+1) + t_{Y \rightarrow X}(n+1)], \quad (36)$$

where ΔS in Eq. (36) equals $\Delta S^{(X, Y)}$. Equation (36) is the analog of Eqs. (9) and (21) within the Liang-Kleeman and Horowitz-Esposito approaches, respectively. We remark that while these analogies are quite illuminating from a thermodynamic standpoint, they must be taken *cum grano salis*. For instance, unlike the information flow $d_t I = \dot{I}^X + \dot{I}^Y$ in Eq. (19), transfer entropy as defined by Schreiber in Eq. (28) is not a flow since it does not add up additively to time derivative of any global quantity. Furthermore, unlike the information flow, transfer entropy is always non-negative. For a recent and detailed information-theoretic analysis on the use of transfer entropy rate and information flow to bound the extracted work during a thermodynamic process with feedback, we refer to [35].

Despite formal mathematical and trivial notational differences, we have provided here a novel quantitative re-examination leading to the essential thermodynamical and physical similarities among the Liang-Kleeman [6], the Horowitz-Esposito [2], and the Schreiber [1] works.

IV. CONCLUSIONS

The stochastic thermodynamical approach to information flows in dynamical systems as presented by Horowitz and Esposito [2] explains that while the second law of thermodynamics is satisfied by the joint system, the entropic balance for the subsystems is adjusted by a term related to the mutual information rate between the two subsystems.

We have conveniently recast the Horowitz-Esposito formalism in Eq. (21) as,

$$d_t S^X + d_t S^Y = d_t S^{XY} + [\dot{I}^X + \dot{I}^Y]. \quad (37)$$

In this article, starting from the conservation of probability and the continuity equation (see Eqs. (1), (3), and (13)), we presented a quantitative discussion on the physical link between the Horowitz-Esposito analysis [2] and the Liang-Kleeman work on information transfer between dynamical system components [6]. In particular, the entropic balance arguments employed in the two approaches were compared. Notwithstanding all differences between the two formalisms, our work strengthens the Liang-Kleeman heuristic balance reasoning by showing its formal analogy with the Horowitz-Esposito thermodynamic balance arguments. We showed that Eqs. (3), (9), and (25) within the Liang-Kleeman approach correspond to Eqs. (13), (21), and (19) within the Horowitz-Esposito approach, respectively. In particular, we have conveniently recast the Liang-Kleeman formalism in Eq. (9),

$$\frac{dH_1}{dt} + \frac{dH_2}{dt} = \frac{dH}{dt} + [T_{1 \rightarrow 2} + T_{2 \rightarrow 1}], \quad (38)$$

and underlined that the sum $T_{1 \rightarrow 2} + T_{2 \rightarrow 1}$ is a flow $d_t I$ in Eq. (25) that adds up additively to the time derivative of mutual information as given in Eq. (22). Finally, we have compared the thermodynamical interpretation of Schreiber's transfer entropy as provided by Prokopenko *et al.* in [25] to both the Liang-Kleeman and the Horowitz-Esposito works. We have conveniently recast the Prokopenko *et al.* formalism in Eq. (36),

$$\sigma^X + \sigma^Y = \Delta S + [t_{Y \rightarrow X} (n + 1) + t_{X \rightarrow Y} (n + 1)]. \quad (39)$$

We provided here a quantitative reexamination leading to the essential thermodynamical similarities among the Liang-Kleeman [6], the Horowitz-Esposito [2], and the Schreiber [1] works. Analogies are summarized in Eqs. (37), (38), and (39).

In synthesis, the main results of our scientific effort can be outlined as follows:

- We established a novel link between the Liang-Kleeman analysis [6] and the Horowitz-Esposito analysis [2] concerning entropic balance arguments in the study of information transfer in complex dynamical systems.
- We strengthened the heuristic Liang-Kleeman information flow analysis [6] with the support of fundamental thermodynamical arguments borrowed from the Horowitz-Esposito work [2].
- We deepened our comprehension of the connection between the (newly thermodynamically grounded) Liang-Kleeman information flow [6] and the thermodynamical analog of Schreiber's transfer entropy [1] as presented by Propokenko *et al.* in [25].

In conclusion, we think that our effort to emphasize such a unifying theoretical picture of thermodynamical nature more or less explicit in different works is extremely important for describing and, most of all, understanding information flows between components of complex systems of arbitrary nature from a foundational point of view.

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